



第201回 OPERA研究交流セミナー
第192回 ISIT有機光エレクトロニクス研究特別室セミナー
第259回 未来化学創造センターセミナー



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②2019年9月27日(金) 10:00~

場所:九州大学 共進化社会システムイノベーション施設 2F 大会議室

Marcus Theory in Electron-Transfer Process

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According to the linear free-energy relationship (LFER), which is the general theory for all chemical reactions, the activation energy (DE_a) decreases with exothermicity of the reaction ($-DG^\circ$); that is, the reaction rate ($\log k$) increases with the ordinal exothermicity of the reaction).

On the other hand, Marcus predicts that the activation energy (DE_a) increases again ($DE_a \propto |DG^\circ|$; $\log k \propto |DG^\circ|$; this region is called as “inverted region”), when the exothermicity exceeds a certain value (= “top region”, $I_{reog} = |DG^\circ|$, I_{reog} is reorganization energy). This Marcus prediction had not been realized experimentally for a long time. However, the Marcus prediction had been realized in some electron-transfer systems as “bell-shape” relation in the $\log k$ vs. $-DG^\circ$ plots, because the electron-transfer rates can be precisely determined for wide-range thermodynamic regions, in which the latter thermodynamic parameters can be evaluated from the redox potentials by the electro-chemical measurements.

In the present seminar, the fundamental of the Marcus theory will be explained with the fundamental of the electron-transfer in both ground-state and excited-state, in which the latter is photo-induced electron-transfer.

In the second day of this seminar, application of the Marcus theory to photo-induced electron transfer systems, because the Marcus theory predicts very fast forward photoinduced-electron transfer in the normal region near the top region ($I_{reog} \sim |DG^\circ|$), while very slow back electron transfer in the inverted region ($I_{reog} \ll |DG^\circ|$). Thus, we can extract separately the hole and electron from the EDA complex (or systems) and use them as further electron and hole mediating systems. Then, such separated electron and hole can be used as solar-cell system, photo-induced hydrogen evolution, photo-synthetics systems (CO_2 -reduction to solar fuels).

Furthermore, in early 21-th century, new carbons such as fullerenes, carbon-nanotubes, carbon nano-horn, single-layer graphene sheet have been applied to photo-induced electron-transfer systems to open “Carbon Photo Science”. Some of such new science will be introduced in this seminar.

主催:九州大学 最先端有機光エレクトロニクス研究センター

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